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Review

Artificial Intelligence for Green Hydrogen Technology and Renewable Energy Integration: A Comprehensive Review

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Abstract- Green hydrogen, produced by renewable energy-powered water electrolysis, is emerging as a promising solution for global decarbonization. Green hydrogen offers a sustainable alternative to fossil fuels, reducing greenhouse gas emissions across various industries. However, several challenges, including energy efficiency, high production costs, and storage concerns, have turned out to be the major impediments to its large-scale deployment. Artificial Intelligence (AI) provides transformative opportunities to optimize green hydrogen production, improve storage techniques, and enable integration with renewable energy systems. This review explores the role of AI techniques, encompassing machine learning, reinforcement learning, and Digital Twins (DTs), in enhancing electrolyzer performance, system degradation prediction, and hydrogen distribution network management. Additional AI applications for storage material discovery, energy forecasting, and sector-level applications in transport, power, and industry are also highlighted in this review. A conceptual framework is provided to map AI models to every stage of the hydrogen value chain. Gaps in the literature and opportunities for interdisciplinary collaboration are identified toward the realization of scalable intelligent hydrogen systems. The review concludes by proposing future avenues for AI-enabled innovations, maintaining a sustainable green hydrogen economy.

Keywords- Green hydrogen; Artificial intelligence; Hydrogen storage; Renewable energy; Water electrolysis; Digital twin

1. INTRODUCTION

Globally, the intensifying climate crisis raised the exigency for transitioning away from fossil fuel-based energy systems towards embracing the production, storage, and consumption of sustainable energy systems. As strategies for decarbonization gain paramount importance in international energy and policy forums, green hydrogen has perpetuated itself as a potential energy security solution. The generation of green hydrogen from the electrolysis of water powered by renewable energy sources is becoming increasingly famous as a clean and scalable energy carrier [1]. Being highly versatile, from energy storage and generation to transportation and industrial processes, convergence with all other forms of clean energy [2]. Compared to blue or grey hydrogen, green hydrogen is carbon-free across its value chain, and as such, it is a key part of the world's decarbonization strategies and a viable vector for incorporating renewable energy sources into multi-sector energy systems [3].

Regardless of its enormous promised potential, the mass deployment of green hydrogen is limited by repeated technological and economic challenges. Those are the high energy requirements of electrolyzer processes, hydrogen storage and transport issues brought about by low volumetric energy density and high diffusivity [4]. In addition, the intermittent nature of renewable energy causes operational instability in hydrogen generation systems, particularly in off-grid or weak-grid settings. Since hydrogen is not just a fuel but also a long-duration energy storage medium, its integration into dynamic energy systems requires smart, real-time optimization of production, storage, and final use applications [5].

To address these challenges, artificial intelligence (AI) is a powerful tool employed to enhance the viability of green hydrogen technologies. AI techniques for green hydrogen automation mainly belong to the category of machine learning (ML) and its subfields like deep learning (DL) and reinforcement learning (RL). Pattern recognition and prediction are the main areas where DL methods such as convolutional and recurrent neural networks are being used, whereas RL is about taking decisions step-by-step and controlling the process in changing operating conditions [6]. In green hydrogen systems, AI algorithms are capable of predicting electrolyzer performance under varying operating conditions, enabling efficient integration with variable renewable energy inputs. Moreover, DTs enable virtual modelling of hydrogen systems, which can be simulated and scenario tested at no physical risk or cost, thus speeding up the innovation cycle.

Although the literature on applying AI systems in energy systems is growing exponentially, most focuses on isolated applications such as hydrogen production or fuel cell control. There is no comprehensive review of AI applications in green hydrogen systems explaining how they are applied in the production, storage, distribution, and sectoral integration. An integrated review is needed to guide interdisciplinary research and enable the design of intelligent, resilient hydrogen infrastructures that are aligned with sustainability goals.

This review attempts to bridge this gap by critically reviewing the state-of-the-art applications of AI across the green hydrogen value chain. It presents a systematic introduction to green hydrogen fundamentals, surveys the AI techniques used, and maps these techniques to related challenges in production, storage, distribution, and end-use. This review explores the technical integration, optimization, and research issues of AI and green hydrogen. It focuses on assessing how AI improves the operation of hydrogen production and storage systems, facilitates renewable energy integration. Through a systems perspective review of these applications, the review points out current limitations, research gaps, and future breakthrough opportunities.

2. AI IN HYDROGEN PRODUCTION SYSTEMS

Green hydrogen is a highly multi-played means of addressing global energy and environmental challenges. Clean and flexible energy carrier capabilities, along with being scalable, place it on the list for future energy systems [2,7]. Hydrogen production through electrolysis is the most pivotal phase of the green hydrogen value chain [8]. Figure 1 depicts the basic architecture of a water electrolyzer system for green hydrogen production. Green hydrogen is mainly generated by water electrolysis, among which the most common methods are alkaline electrolysis (AEL), proton exchange membrane electrolysis (PEM) and solid oxide electrolysis cells (SOEC). AEL is a well-established, economical method; PEM has the ability to provide high current density and rapid dynamic response; and SOEC is the technology that operates at high standards of electricity and thus achieves higher efficiency when paired with waste heat sources [9,10]. Nonetheless, real-world deployment of these systems is limited by several factors, such as high energy consumption, sensitivity to fluctuating operational conditions, and degradation of key components over time.

Concerning the green hydrogen economy, there are two significant limitations at present. Primarily, there is an energy-intensive process inherent in electrolysis. Conventional control techniques in electrolyzers, employing fixed-rule-based logic and manual optimization, tend to be unable to respond to these dynamic and nonlinear operational conditions. This introduces inefficiencies in energy usage, hydrogen production, and system lifespan [11]. Also, the cost of capital required for the electrolyzer unit and the renewable energy generation system, together with the cost of auxiliary infrastructure, is very high. Presently, the Levelized Cost of Hydrogen (LCOH) for green hydrogen tends to be more than the LCOH of grey or blue hydrogen, though this is expected to shrink due to better policy incentives, technological improvements, and scaling [12]. Hydrogen production is complicated by the intermittent and variable nature of renewable energy sources, leading to less consistent and less reliable hydrogen output. Operational stability is further compromised in off-grid or weak-grid regions, specifically when hydrogen production systems are operated adjacent to Distributed Energy Resources (DERs).

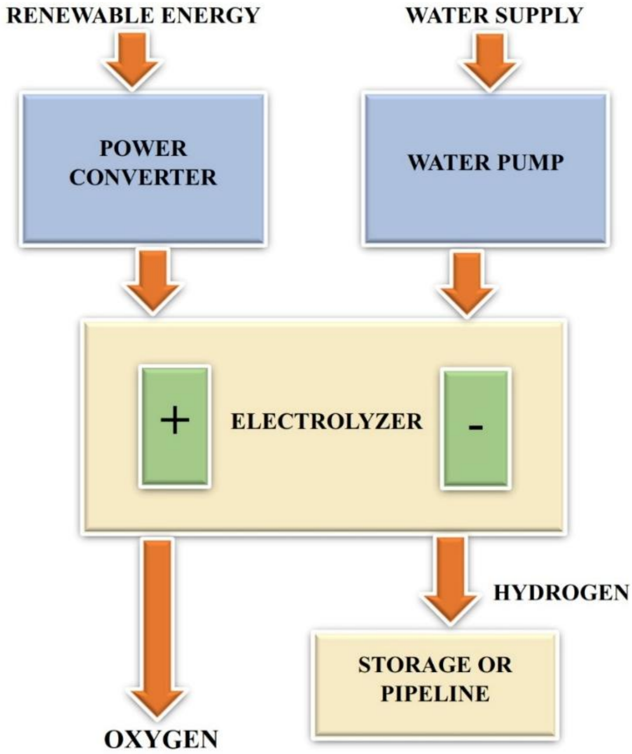

Figure 1. Basic Architecture of a Water Electrolyzer System for Green Hydrogen Production

Hydrogen poses unique problems in storage and transport, given its low-energy-density volume and high diffusivity. Storage technologies are supposed to resolve issues such as material embrittlement, energy-intensive compression, and/or cryogenic liquefaction [13]. Green hydrogen for industrial facilities like steelworks, ammonia production, and refining shall be a promising path for decarbonization [14]. Traditionally, these industries have been difficult to electrify, yet they are big carbon emitters. Hydrogen replaces fossil fuels in industries as a feedstock and energy source for high-temperature processes. On the transportation front, hydrogen Fuel Cell Vehicles (FCVs), in turn, will provide long-range, fast refuelling alternative solutions to battery-electric vehicles, mainly for heavy-duty uses [15,16]. Table 1 presents a comparative summary of the key hydrogen production technologies to show the differences in the energy source, emissions, efficiency, and cost for grey, blue, and green hydrogen, respectively.

Artificial intelligence holds great potential in optimizing hydrogen production through data-driven modelling, adaptive control, and predictive diagnostics [17]. Some of the popular AI techniques used in the field are supervised machine learning methods, including artificial neural networks (ANN), support vector machines (SVM), and Random Forest Regressors [18,19]. They are trained on electrolyzer operating data, including current density, temperature, voltage, membrane hydration, and gas purity. Energy Management Systems (EMS) provide another example of AI integration. Artificial intelligence is a boon, enabling systems control in real time, predictive diagnostics, operational optimization, and digital simulation [20]. AI integration with electrolyzer systems thus converts these static, energy-intensive units into adaptive, highly-intelligent assets capable of functioning efficiently under different environmental and load conditions [21]. AI algorithms optimize the energy flow in real time, and keep generation in balance with consumption [22]. Through understanding nonlinear relationships between such parameters, AI models can make predictions about optimal setpoints for maximum hydrogen production with minimum energy losses. This strategy makes real-time adaptation to power input fluctuations from non-dispatchable renewable resources like solar and wind possible, which are responsible for destabilizing the efficiency of electrolyzers if not addressed carefully [23,24]. Machine learning methods enable dynamic optimization by learning and adapting to the nonlinear relationship between input parameters and efficiency [25]. AI assists with the integration of renewable power sources into the grid. The inherent variability of wind and solar power generation scale requires accurate forecasting coupled with real-time balancing mechanisms. Hybrid AI models are developed and utilized to forecast renewable energy output with improved accuracy by combining meteorological data, satellite images, and historical performance records. AI-controlled dispatch and storage may be adjusted in real-time to help regulate voltage and frequency variations [26]. Figure 2 depicts a simplified flow chart that describes how AI interacts with renewable energy systems to enable intelligent forecasting, control, and optimization.

Table 1. Comparative overview of hydrogen production methods

Parameter	**Grey Hydrogen**	**Blue Hydrogen**	**Green Hydrogen**
Primary Energy Source	Natural gas (fossil fuel)	Natural gas + Carbon Capture	Renewable energy (solar/wind)
Production Technology	Steam Methane Reforming (SMR)	SMR + Carbon Capture and Storage	Water electrolysis
CO_2 Emissions	High	Moderate (depends on CCS rate)	Near zero
Energy Efficiency (%)	~65-75	~60-70	~60-70 (improving with PEM/SOEC)
Cost (USD/kg)	~1.0-1.5	~1.5-2.0	~3.0-6.0 (location dependent)
Maturity Level	Commercial	Emerging	Emerging/R&D
Key Challenges	Emissions	CCS cost & leakage	High cost, intermittency

Reinforcement learning (RL) brings with it another promising perspective, allowing electrolyzers to learn by themselves some control policies that may help them maximize performance in the long run. In contrast to supervised learning, wherein the learner utilizes historical data with relevant labels, RL agents interact with the system environment and modify their actions according to feedback. Such feedback is indicated through a reward function, such as a reward which might be hydrogen output per unit of energy input. Because of this ability, RL becomes very effective in systems with fluctuating inputs or uncertain operating conditions, typical in distributed renewable energy settings [27]. Simulation studies in recent years have indicated that RL methods, when informed by grid-side dynamics and short-term weather patterns, can achieve considerable reductions in energy consumption [28].

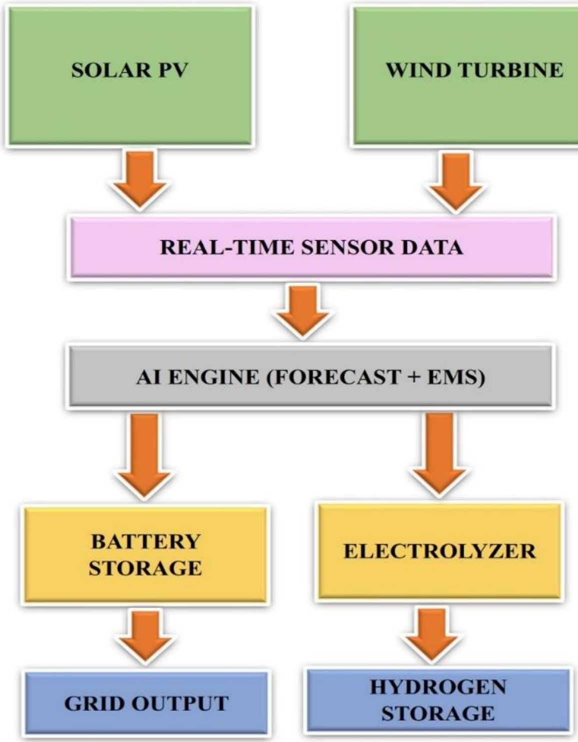

Figure 2. AI Integration Flow in Renewable Energy Systems

Figure 3 portrays the architecture of an AI-supported electrolyzer system and emphasizes sensor integration, real-time control loops, and predictive analytics modules. In Figure 3, the structure of an AI-assisted electrolyzer monitoring and control system is shown, consisting of the immediate sensor data going through the machine learning and reinforcement learning models. The AI layer adds predictive analytics, adaptive control, and fault detection to enhance electrolyzer efficiency, reliability, and operational lifetime with changing renewable energy inputs.

Apart from performance optimization, AI-based systems also play a role in the predictive maintenance of electrolysis systems. Ageing of an electrolyzer can be due to catalyst poisoning, membrane thinning, or gas crossover, each of which compromises the system's efficiency and increases downtime. Deep learning methods, including convolutional neural networks (CNNs) and long short-term memory (LSTM) networks, have been heavily relied upon in green hydrogen systems for tasks such as pattern recognition, fault detection, and time-series forecasting. CNNs are largely utilized for the extraction of spatial attributes and detection of anomalies, whereas LSTM networks excel in capturing the temporal relationships in the data of renewable generation and system performance [29,30]. This implies predictive diagnosis, where one arranges maintenance on a proactive basis according to the estimated remaining useful life (RUL). This minimizes operational risks and maintenance costs [31].

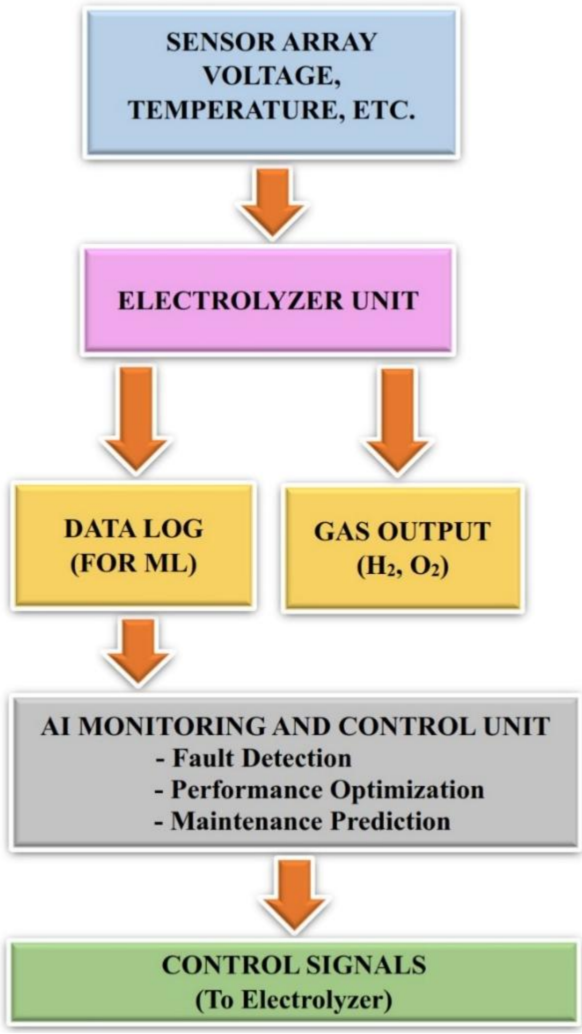

Figure 3. AI-Enabled Electrolyzer Monitoring and Control System

Explainable artificial intelligence (XAI) implicates a set of methods that assist in understanding the decision-making process of machine learning models through providing human-like explanations of the predictions made by the models. The use of XAI in green hydrogen systems is of utmost importance in safety, regulatory compliance, and building operator trust in AI-supported control and decision-making. XAI techniques, encompassing SHAP (Shapley Additive Explanations) and LIME (Local Interpretable Model-Agnostic Explanations), can be implemented to interpret outputs from models, thereby giving industrial operators confidence and transparency in AI-based decision-making [32,33]. Table 2 lists some of the most prominent AI methods applied in the optimization of electrolyzer performance, their areas of application, advantages, and examples of use.

Table 2. Summary of AI Techniques in Electrolyzer Optimization

AI Technique	Application Area	Benefits	Example Use Cases
Artificial Neural Networks (ANN)	Electrolyzer performance modelling	Predict hydrogen output, energy use	Forecast voltage/current behaviour
SVM	Fault detection and diagnostics	Classify operating states	Detect membrane degradation
RL	Real-time operational control	Adaptive control under uncertainty	Optimize setpoints with variable input
DTs + ML	Simulation and virtual optimization	System design and degradation tracking	Predict ageing trends, what-if analysis
Random Forests / Gradient Boosting	Multi-parameter optimization	Identify optimal conditions	Electrolyte temp/current tuning

Forecasting models provide forecasts of renewable energy generation from weather data, and load-shifting strategies usher in low-price electricity hours completed from grid electricity during high-price hours [34]. Bayesian optimization and genetic algorithms are some of the tools used to target optimal parameter combinations amid trade-offs between efficiency, cost, and system wear. In addition, AI can be used to promote Demand Side Management (DSM) with hydrogen production embedded into large smart grid frameworks. In such a framework, hydrogen production acts as a flexible load to absorb overt renewable energy, thereby stabilizing the grid and minimizing curtailment losses. AI-based control algorithms manage this interaction by forecasting demand, predicting grid conditions, and adjusting hydrogen output dynamically.

Digital twins (DTs) technology further enhances AI capabilities in hydrogen production. Essentially, a DTs stands for a virtual replica of the physical electrolyzer system that is continuously updated with newer real-time operational data [35]. The AI models embedded within the DTs simulate thermodynamic, electrochemical, and mechanical behaviour under various operating scenarios. This enables system operators to conduct "what-if" tests, validate new control strategies, and optimize component design, all while the real system continues to operate [36]. DTs lengthen system life, help to achieve virtual commissioning of new components, and train operators. They are also platforms to validate AI algorithms to test novel control schemes given simulated conditions before deployment into the physical world. During pilot projects in Europe and Japan, DTs integrated with AI showed features that could potentially extend their use and improve fault detection [37]. Such projects emphasize that AI applications are feasible and beneficial, whereas wide adoption fails because of barriers like data quality, system interoperability, and capital investment [38].

The aim of incorporating AI into green hydrogen production is to address major practical challenges to system efficiency, reliability, and cost. Integrating AI into hydrogen production systems does present some challenges. Data quality and availability remain the bottlenecks, especially for pilot systems with limited historic workability. In addition, computational costs, interpretability of models, and interoperability considerations between various hardware and software platforms may also hinder deployment [39]. However, with edge computing, federated learning, and open data platforms now in the forefront, all these challenges are getting sufficiently addressed. Through applications of predictive modelling, adaptive control, and virtual simulation, AI removes the element of human decision-making from every step of the production process. As AI technology advances, hydrogen production stands to grow more capable, data-centric, and critical to future energy systems.

3. AI IN HYDROGEN STORAGE AND DISTRIBUTION

Effective storage and transportation are critical to the potential of green hydrogen as a full-scale energy carrier. Very low volumetric energy density, high diffusivity, and flammability in hydrogen storage pose major technical challenges compared to traditional fuels. Each storage method, carries its trade-offs concerning the density of energy, thermal dissipation, and incompatibility with certain materials. The design of hydrogen pipelines, fuelling stations, and distribution networks must account for allowing very little loss and ensuring safety. Artificial Intelligence (AI) has proven to be a key driver for optimizing the performance, safety, and economic efficiency of hydrogen storage and distribution networks through real-time monitoring, intelligent control, and system-level optimization. Implementation of AI in hydrogen storage starts with the discovery and selection of materials [40].

AI techniques have been used increasingly in the modelling and prediction of complex storage system behaviour in hydrogen storage. Amongst the modern hydrogen storage materials, one of the most promising avenues opened up is via metal-organic frameworks (MOFs) that have attracted considerable interest for their high surface area, adjustable pore structure and possible increase in hydrogen adsorption. MOFs allow for systematic investigation of structure-property relationships and data-based and ML methods are frequently used for the optimization of hydrogen storage performance. Historically, the discovery of materials has depended heavily on slow and computationally intensive quantum mechanical calculations. In contrast, supervised learning models learn from experimental and simulation data sets and forecast material properties like adsorption capacity, reaction enthalpy, and cycle stability accurately. This saves time and expense in experimental screening and allows high-throughput investigation of material libraries [41].

AI can monitor tank performance, detect leakage, and optimize thermal management in gaseous and liquid-hydrogen storage systems. Neural networks and decision tree algorithms can be trained to detect anomalous temperature and pressure patterns that foreshadow failures in storage systems. They utilized to implement adaptive control strategies that could manage the boil-off rate in cryogenic storage tanks, thereby optimizing both energy consumption and operational safety. In mobile applications, AI systems dynamically control tank pressure and flow rates of hydrogen to the fuel cell stack in real time, based on driving conditions and energy requirements. AI is also vital in monitoring and controlling the operational features of hydrogen storage systems. Real-time data acquisition from pressure sensors, temperature probes, and flow meters produces high amounts of heterogeneous data that need to be processed quickly to ensure safe and efficient operation. AI methods like anomaly detection, clustering, and predictive analytics are used to detect possible faults, pressure accumulation, or thermal hotspots. These models allow for pre-emptive corrective measures, thus improving system safety and reliability [42]. In Figure 4, the optimization of the hydrogen storage and distribution value chain, from leak detection to routing logistics, with AI, is illustrated. In Figure 4, the pipeline of AI-assisted hydrogen storage and distribution is depicted, showcasing the use of machine learning and optimization algorithms for leak detection, safety monitoring, and logistics planning. The use of AI analytics facilitates the routing, decision-making, and operation across the hydrogen storage and transportation infrastructure to be efficient, instant, and reliable.

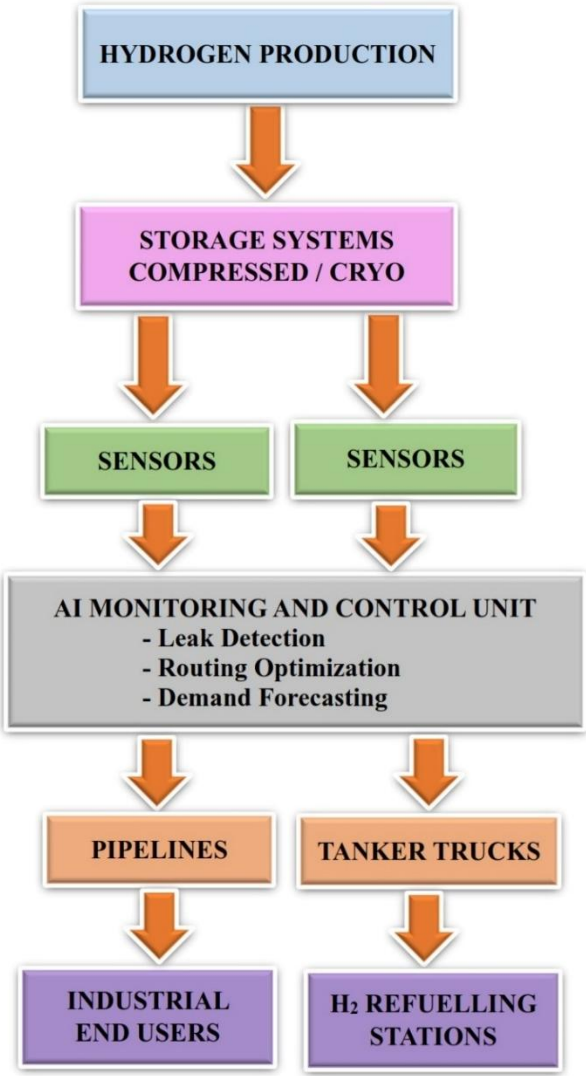

Figure 4. AI-Assisted Hydrogen Storage and Distribution Pipeline

Among the distribution systems, the first use of AI is for logistic management and infrastructure planning of hydrogen supply chains. Optimization algorithms can set into relation spatially and temporally hydrogen demand to assist with strategic location decisions of refuel stations, and scheduling of deliveries by truck or ship [43]. Such coordinated management minimizes curtailment losses and enhances the overall efficiency of the green hydrogen value chain [44]. Reinforcement learning has been suggested for dynamic route optimization, where hydrogen delivery is dynamically adjusted in real-time based on traffic, weather, or grid demand patterns. These methods would help keep operational costs low while honouring time-bound delivery constraints that are very important in integrating hydrogen at a large-scale level into the urban energy network [45].

In addition, DTs of hydrogen storage and distribution networks are a strong tool for real-time analysis and decision-making. DTs include sensor data in tanks, compressors, valves, and pipelines and model their physical behaviour under different operating conditions. AI models in the DTs framework identify performance loss, model emergency response planning, and provide preventive recommendations. In massive hydrogen hubs or export terminals, DTs with AI integration have been employed to model and manage interactions among storage, liquefaction, compression, and export facilities to enhance total system efficiency and resiliency [46]. The existing storage methods of hydrogen and the functionalities given by AI-enhancements are briefly outlined in Table 3 in such a way as to indicate the avenues through which AI can work on bettering performance, safety, and material innovation.

Table 3. Comparison of Hydrogen Storage Technologies Enhanced by AI

Storage Method	AI Application	Key Benefits	Limitations
Compressed Gas	Leak detection, pressure prediction	Improved safety, predictive alerts	High energy for compression
Liquid Hydrogen	Cryogenic control optimization	Temperature stability, loss minimization	Boil-off, energy intensity
Metal Hydrides	Material discovery via ML	Enhanced capacity, kinetics	Heavy, thermal management
MOFs/Porous Materials	Adsorption behaviour prediction	Screening of novel materials	Expensive synthesis, lower densities
Chemical Carriers	Reaction pathway modelling	Efficient synthesis and decomposition	Complex regeneration

Still, several challenges need to be overcome to realize the optimal deployment of AI in hydrogen storage and distribution. These include high-fidelity sensor inputs, data protocols standardization, cyber-physical security, and explainability of AI decisions in infrastructure systems [47]. The integration of physics-informed machine learning models, which infuse conservation laws and physical constraints into AI models, holds a promising future for improving model reliability in storage systems. In addition, cross-sector cooperation and the creation of open-access data sets will be necessary for training strong models and encouraging the uptake of AI throughout the hydrogen supply chain. Overall, the application of AI in hydrogen storage and distribution networks is promising to break the traditional technical barriers. Through predictive monitoring, logistics optimization, and material discovery acceleration, AI can increase the safety, efficiency, and scalability of hydrogen infrastructure, facilitating its expanded use in a decarbonized energy future.

4. AI FOR THE INTEGRATION OF HYDROGEN WITH RENEWABLE ENERGY SYSTEMS

The efficient incorporation of green hydrogen production in renewable energy systems is crucial in the realization of a flexible, decarbonized energy system. Hydrogen serves as a chemical energy carrier that helps balance out the intermittency of renewable sources like solar and wind, facilitating energy storage, sectoral coupling, and long-term grid stability [48]. But such integration presents tough problems, among which are supply and demand profile mismatches, real-time control of electrolyzers under changing inputs, and multi-energy system co-optimization. Artificial intelligence has proved to be a driver in resolving these issues, providing adaptive, data-driven solutions to system-level control, prediction, and energy management.

One of the fundamental prerequisites for successful integration is reliable forecasting of renewable generation. AI-based prediction and forecasting are among the most advanced and influential uses of renewable-hydrogen integration. Precise short-term and long-term solar irradiance prediction, wind speeds, electricity prices, and hydrogen demand are vital for scheduling electrolyzer operation, storage use, and power dispatching. Machine learning algorithms like Support Vector Regression (SVR), Artificial Neural Networks (ANN), Gradient Boosting Approaches, and Hybrid Ensemble Methods have been extensively employed to perform these functions. These models train on intricate temporal and spatial patterns from past meteorological and system histories with higher accuracy than traditional statistical techniques [49]. Recent applications have illustrated that deep learning architectures, specifically CNNs, Recurrent Neural Networks (RNN) and LSTM networks, deliver improved performance in multi-step time series forecasting of renewable generation and hydrogen demand profiles [50]. Besides forecasting, AI facilitates real-time load management and energy dispatch.

In real-time control systems, AI helps maintain the optimal functioning of hybrid energy systems consisting of renewables, hydrogen electrolyzers, fuel cells, and battery storage. Rule-based control is usually inadequate for high-dimensional, nonlinear dynamics of such systems, particularly under fluctuating renewable input. By contrast, machine learning-powered control strategies such as model predictive control (MPC) with machine learning surrogates, reinforcement learning agents, and fuzzy logic controllers optimize the system parameters in real-time to maximize overall efficiency. A reinforcement learning algorithm can learn to optimize electrolyzer load based on forecasted solar output and electricity prices, maximizing hydrogen production while lowering operational expenses and grid stress. Table 4 compares the leading electrolysis technologies and the AI solutions developed to overcome their operational challenges.

In systems where hydrogen is used as both storage vector and energy carrier, AI plays a crucial role in managing bidirectional energy exchange between renewable sources, hydrogen production, and reconversion technologies like fuel cells or gas turbines [51]. A block-diagram representation of the hybrid EMS incorporating AI, renewables, and hydrogen infrastructure is depicted in Figure 5. An AI-driven EMS that incorporates renewable energy sources along with hydrogen production, storage, and use is depicted in Figure 5. The diagram illustrates the way in which the AI-based predictions, optimizations, and instantaneous control are synchronizing the energy movements between the electrolyzers, batteries, and the grid. This smart conducting of energy flow, in turn, improves the efficiency, flexibility, and reliability of the system even in times of fluctuating renewable power generation. The idea of hydrogen as a grid-balancer is gaining wide popularity. During surplus renewable generation, AI can divert excess electricity to water electrolysis, and the energy can be stored as hydrogen. During peak demand or low renewable generation times, stored hydrogen can be converted into electricity, fed into the grid, or used in industrial processes.

Table 4. Comparative Overview of Electrolysis Technologies and Associated AI Applications

Electrolysis Type	Key Features	Operational Challenges	AI Application Area	Sample AI Methods	Ref.
AEL	Mature, low-cost	Slower response to load variation	Efficiency prediction, fault detection	ANN, SVM	[52]
PEM	Fast response, high-purity hydrogen	High cost, catalyst degradation	Load control, predictive maintenance	RL, CNN	[53]
SOEC	High efficiency, operates at high temperature	Thermal stress, material instability	System modelling, degradation monitoring	Physics-informed ML, LSTM	[54,55]

AI provides the best timing and quantity for such conversions by considering real-time grid conditions, economic indications, and technical limitations. Such flexibility increases the reliability of the energy system and facilitates the integration of greater percentages of variable renewables [40]. Energy system modelling and multi-objective optimisation have emerged as major areas of application for AI tools in system planning. These techno-economic analyses find the uses of genetic algorithms, particle swarm optimisation, and deep reinforcement learning in optimising the sizing and siting of hydrogen production units over spatial and temporal scales [56]. Thus, different constraints can be considered, including land availability, grid capacity, CO_2 emissions, and economic returns. Within integrated energy systems or energy communities, AI is employed to coordinate interactions between electricity, gas, and thermal systems for sector coupling-enhancing flexibility and resilience of the overall energy system.

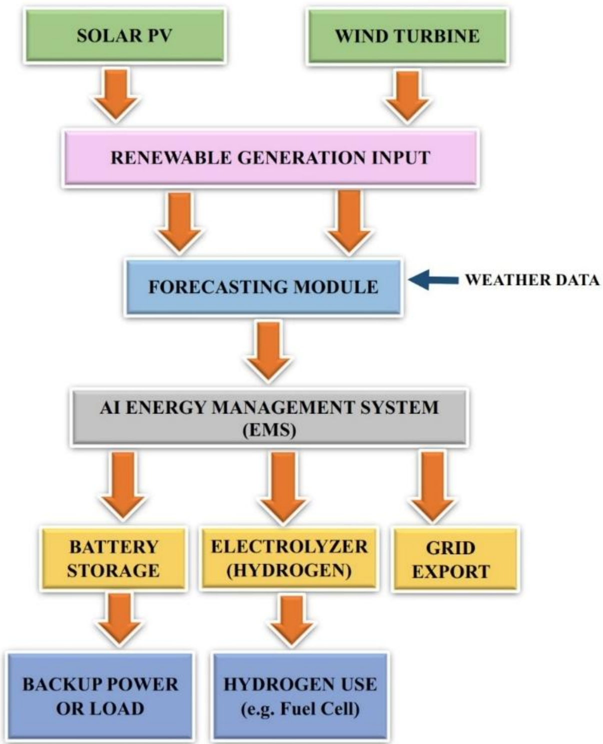

Figure 5. EMS Integrating Renewables, AI, and Hydrogen

Another trending subject is AI and DTs-driven energy management. The system keeps perpetually updating a real-time or DTs of the whole renewable-hydrogen setup through sensor data and operational feedback [57]. Embedding the AI models in this platform helps to simulate various operational conditions, predict disturbances, and support decision-making for operators and automated control agents. In the virtual power plant mode of operation, it coordinates distributed renewable generators, for electricity market participation, peak demand management, and provision of ancillary services [58]. Table 5 presents the major artificial intelligence methods used in different parts of green hydrogen systems, their functional roles, advantages, and disadvantages. However, these developments still have constraints and challenges to contend with. Lack of standard protocols that allow interoperability among heterogeneous hardware and software systems is still a huge subject to explore. For real-world deployment, AI models should be robust to uncertainty and fully operational under incomplete or noisy data. Inserting physics-based constraints into AI models constitutes a promising avenue for reliability and interpretability enhancement, otherwise referred to as physics-informed machine learning.

Table 5. AI Techniques and Their Applications in Hydrogen Systems

AI Technique	Application Area	Input Features	Target Output	Benefits	Limitations
ANN	Electrolyzer performance prediction	Voltage, current, temperature, membrane hydration	Hydrogen yield, system efficiency	Nonlinear modelling, fast adaptation	Requires large datasets, black-box nature
SVM	Fault detection, gas purity control	Sensor signals, operating pressure	Fault classification	High accuracy with small datasets	Less effective on noisy data
RL	Dynamic load control	Real-time renewable generation, price signals	Optimal control policy	Learns through interaction, handles uncertainty	High training time, exploration risks
CNN	Anomaly detection in electrolyzers	Time-series or image-based diagnostics	Maintenance alert, degradation patterns	High feature extraction capability	Requires labelled failure data
Genetic Algorithms (GA)	Storage optimization, route planning	System constraints, storage capacity, distances	Optimal storage layout, delivery schedule	Solves multi-objective problems	May converge slowly

Moreover, ensuring cybersecurity in AI-managed hydrogen systems is important to ensure critical infrastructure protection from data breaches and adversarial attacks. To sum up, artificial intelligence plays an ever more pivotal role in facilitating the integration of hydrogen into renewable energy systems. With forecasting, control, and optimization functions, AI helps ensure the stability, efficiency, and scalability of renewable-hydrogen hybrid systems and thus promotes the worldwide shift toward sustainable and intelligent energy infrastructures.

5. SECTORAL APPLICATIONS AND DIGITAL INFRASTRUCTURE OF AI-DRIVEN HYDROGEN SYSTEMS

Green hydrogen coupled with artificial intelligence has the potential to change many heavy energy-intensive sectors for operations and accelerated processes of developing intelligent infrastructure. Some of these promising sectors that exhibit the most opportunities with this synergy are transportation, power generation, and industrial manufacturing. Embedding AI in these sectors increases the operational scope and strategic value of hydrogen as a foundation for sustainable energy transitions. At the same time, the digital infrastructure for these applications is essential in ensuring system-wide integration, coordination, and scalability [39].

In the transportation industry, hydrogen presents a promising pathway as a low-carbon substitute for fossil fuels in heavy-duty trucks, trains, and shipping. The adoption of AI in hydrogen-powered transport systems enables smart fuel cell management, route planning, and refueling operations. Onboard AI systems can forecast energy demand from driver behaviour and ambient conditions, allowing adaptive control of the fuel cell to maximize efficiency and extend component life. Fleet-level AI systems apply real-time traffic, weather, and demand information to optimize dispatch and refueling schedules for vehicles, balancing hydrogen supply with consumption requirements while reducing wait time and infrastructure stress. AI helps optimize hydrogen vehicle performance via predictive diagnostics, route planning, and energy management [59]. In urban mobility networks, hydrogen buses and delivery fleets, AI systems combine transportation information with hydrogen availability to schedule operations and minimize emissions efficiently [60,61].

In the power generation industry, hydrogen is used as a long-duration energy storage medium and a flexible generation resource. Hydrogen acts as an adaptive energy carrier that can store excess renewable electricity and deliver power in the form of fuel cells or gas turbines during peak demand [62]. AI-powered EMS can manage the interactions between hydrogen storage facilities, renewables, offering load balancing, peak shaving, and frequency regulation services [58]. These systems utilize predictive analytics and optimization algorithms to calculate the most economical and sustainable utilization of stored hydrogen during real-time operations. Furthermore, AI is capable of augmenting economic dispatch models that calculate when to run hydrogen-based generators in terms of electricity prices, demand forecasts, and carbon intensity targets. AI enables the smooth operation of such systems by predicting power demand, renewable generation, and hydrogen supply. Power-to-Gas-to-Power (P2G2P) systems are those that transform renewable electricity into hydrogen and this hydrogen can be stored to be reconverted back to electricity in times of necessity. Implementation of AI-based optimization and control techniques not only increases the energy efficiency and flexibility of the P2G2P systems but also makes the system more cost-effective in the energy integration scenario. RL and optimization models select the least expensive times to convert electricity to hydrogen and back, taking into account electricity market prices, storage levels, and the need for grid balancing. These features allow power systems based on hydrogen to offer ancillary services like frequency regulation, voltage support, and spinning reserve, which will make the grid more reliable and stable [63].

In microgrids and remote energy, hydrogen supplements solar photovoltaics and wind power through seasonal energy storage as a buffer. AI harmonizes the relationship between renewable power generation, battery storage, and hydrogen conversion units to provide an uninterrupted energy supply in remote areas. Predictive models evaluate weather conditions, load profiles, and energy consumption behaviour to adjust hydrogen production and reconversion strategies in advance. These uses are especially important in island economies, remote communities, and disaster zones, where energy independence and resilience are of prime importance.

In commercial uses, especially in industries like steel production, ammonia production, and petrochemicals, hydrogen is being contemplated as a green feedstock to substitute for carbon-based processes. In these applications, AI can be utilized to track and optimize the flow, pressure, and purity of hydrogen in real-time at maximum efficiency. Machine learning-augmented process control models can forecast equipment breakdowns, and automate real-time process parameter adjustments based on process-level feedback [43]. AI improves industrial utilization of hydrogen by maximizing combustion management, process integration, and logistics in supply chain management [64]. Additionally, AI can support Life-Cycle Assessment (LCA) models by dynamically merging process-level data to analyze the carbon footprint and sustainability of hydrogen use throughout industrial value chains.

Table 6. Sectoral Applications of Hydrogen and AI Integration

Sector	Hydrogen Application	AI Application Areas	Specific AI Algorithms	Key Benefits
Transportation	Fuel for fuel-cell vehicles (buses, trucks, trains, shipping)	Fleet management, route optimization, fuel cell control, predictive maintenance	ANN, LSTM (energy demand prediction); RL (route and powertrain optimization); SVM (fault detection); Genetic Algorithms (fleet scheduling)	Improved fuel efficiency, reduced downtime, optimized refuelling, lower emissions
Power Generation	Long-duration energy storage, grid balancing, P2G2P systems	Load forecasting, energy dispatch, ancillary services, peak shaving	LSTM, CNN (load and renewable forecasting); Reinforcement Learning (dispatch optimization); Model Predictive Control (MPC); DTs (system simulation)	Enhanced grid stability, renewable curtailment reduction, improved reliability
Industry	Feedstock and high-temperature heat (steel, ammonia, methanol, refining)	Process control, combustion optimization, anomaly detection, predictive maintenance	ANN, Random Forests (process optimization); CNN (anomaly detection); Physics-informed ML (process modelling); XAI (decision transparency)	Emissions reduction, energy savings, improved process efficiency
Buildings	Backup power, combined heat and power (CHP), heating	Demand forecasting, smart energy management, load shifting	ANN, LSTM (demand prediction); Fuzzy Logic Controllers; Reinforcement Learning (energy management)	Load optimization, peak shaving, reduced energy costs
Hydrogen Supply Chain	Production–storage–distribution coordination	Logistics optimization, demand forecasting, safety monitoring	Genetic Algorithms (routing and scheduling); Multi-agent RL (supply coordination); SVM, CNN (leak detection); DTs (infrastructure planning)	Improved efficiency, enhanced safety, cost reduction, supply reliability

Supply chain management and hydrogen logistics are also augmented with AI. Complex planning and dynamic adjustments in coordination are necessary to schedule hydrogen production, storage, and consumption between geographically dispersed locations. AI systems track patterns of demand, infrastructure capacity, and availability of transport to formulate the best supply chain routes. Such models are implemented using real-time limitations such as weather impact, equipment schedules, and energy costs to update delivery timing and stock levels. Digital platforms supported by AI allow stakeholders to visualize and manage the hydrogen value chain, enhancing responsiveness and transparency [65]. Hydrogen can be utilized in combined heat and power (CHP) systems, fuel cell-based backup power systems, and heating appliances in the built environment.

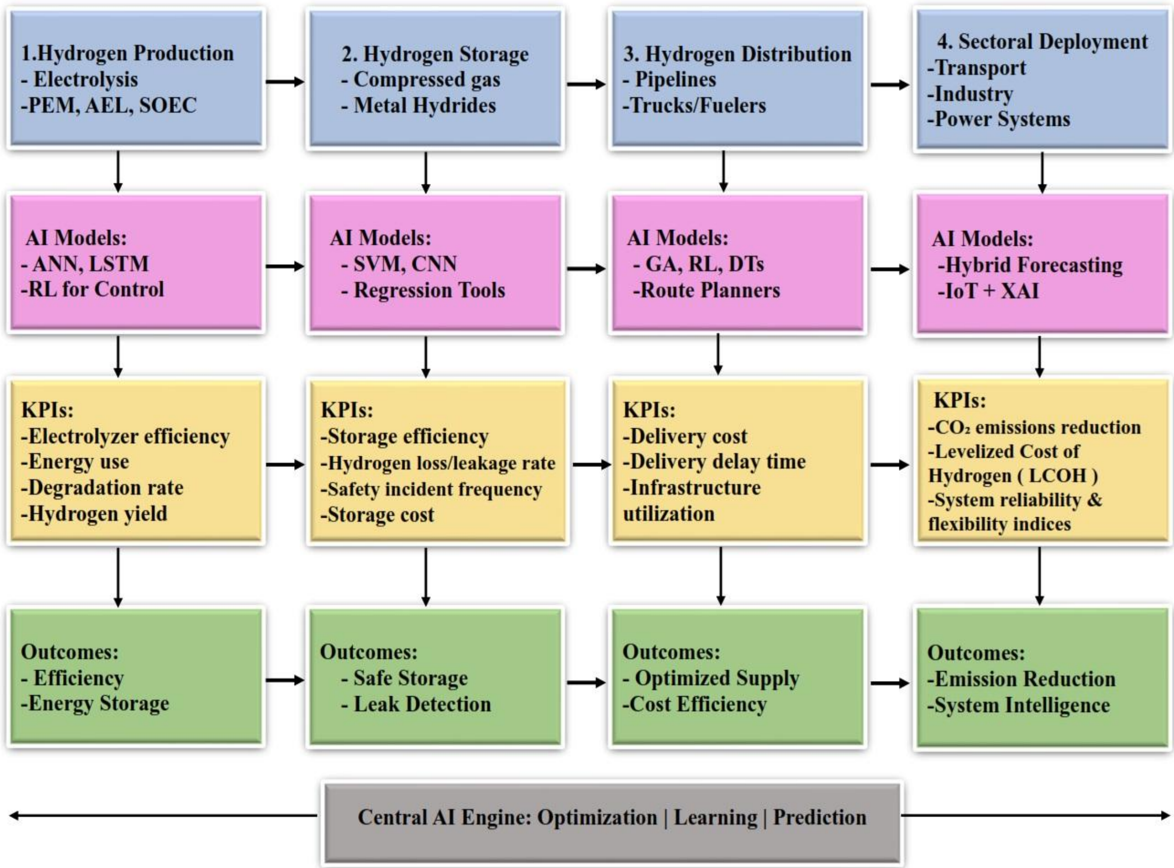

Figure 6. Actionable Framework for AI Integration in the Green Hydrogen Value Chain

AI offers the intelligence to enable hydrogen technologies to be integrated easily into existing infrastructure, and coordinate their operation with overall energy system goals. These uses highlight the function of AI not only as an adjunct tool but also as a key enabler of hydrogen's systemic integration [66]. Table 6 provides a high-level overview of green hydrogen applications across sectors and related AI tools for system efficiency, reliability, and integration. Figure 6 presents a conceptual framework illustrating how artificial intelligence technologies are integrated across the green hydrogen value chain, from production and storage to distribution and sectoral deployment.

It demonstrates the deployment of artificial intelligence throughout the green hydrogen value chain, identifying top technologies, AI approaches, and their respective benefits at each step. At each stage, the representative AI methods are connected with operational functions and measurable performance indicators, thus allowing for production, storage, distribution, and system-level integration to be supported by actionable decision-making.

Behind all these applications is the increasing role of resilient Digital Infrastructure, which serves as the foundation for data acquisition and control within hydrogen systems. Internet of Things (IoT), 5G, cloud computing, and edge computing platforms together facilitate real-time data transmission and processing across distributed hydrogen assets [67]. AI systems are installed both in cloud-based control centres and on edge devices integrated with physical infrastructure, enabling decentralized intelligence and quick response times. DTs, as mentioned above, are increasingly employed to model entire sectoral systems like a hydrogen refueling infrastructure or a hydrogen-powered microgrid, enabling real-time simulation, optimization, and diagnostics [68]. Figure 7 depicts the architecture of a DTs system integrated with AI for monitoring and optimizing hydrogen production in real time. Sensor data is constantly fed from the physical system to the virtual model for predictive diagnostics, performance optimization, and what-if analyses. With a handful of sensors for system-side or process-side control, this AI-facilitated DTs is expected to improve hydrogen systems by enabling informed decisions, preventing faults, and operating with greater efficiency.

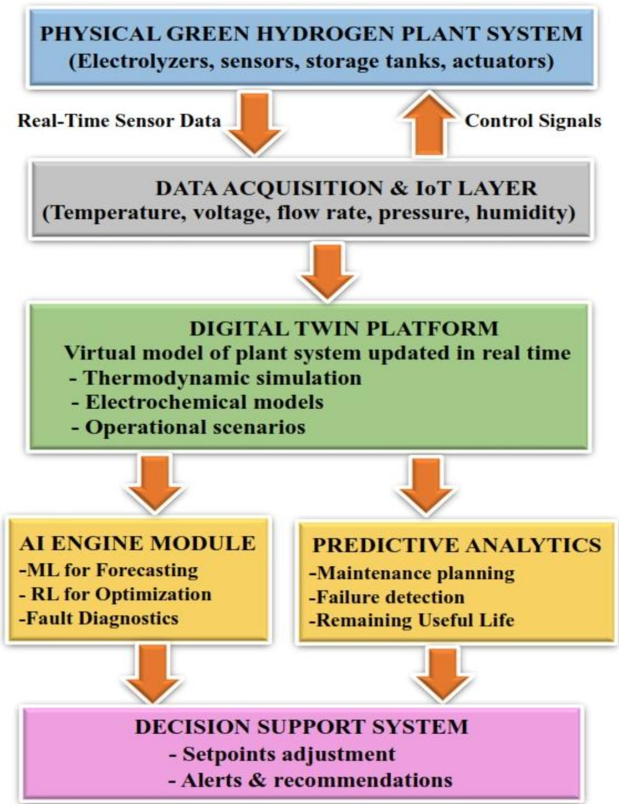

Figure 7. Digital Twin Architecture for an AI-Enhanced Green Hydrogen Plant

Cybersecurity and data privacy are serious issues in the implementation of digital infrastructure for hydrogen systems, particularly as these systems become more integrated and dependent on AI. Securing AI models and communication channels against adversarial attacks is necessary to guarantee the dependability and safety of hydrogen-fuelled systems. Secure AI architectures and resilient digital platforms that can identify anomalies, and recover from interruptions without system failure are being developed. Together, the combination of artificial intelligence, digital infrastructure, and hydrogen applications across sectors is a frontier of innovation that enables high-emitting sectors to decarbonize. Through AI-powered smart system design and coordination, hydrogen transitions from the lab bench into real-world, scalable technologies in transportation, power, and industry, enabling a cleaner, more resilient energy future.

6. CHALLENGES, RESEARCH GAPS AND FUTURE SCOPE

Although the synergy of artificial intelligence and green hydrogen is very promising for decarbonizing energy systems, various technical, infrastructural, and institutional barriers impede the complete unfolding of this synergy. These barriers cut across data availability, model resilience, system integration, standardization, and scalability. They need to be overcome through concerted interdisciplinary research, policy guidance, and cross-sectoral collaboration [69]. One key limitation in all hydrogen production, storage, and distribution systems is the scarcity and fragmentation of high-quality and labelled data sets. Supervised learning-based AI models rely heavily on quantities of past operational data for training, testing and validation [46]. Yet, numerous hydrogen systems are still in pilot or demonstration form, thus restricting real-time data streams. Even where data are available, they tend to be isolated within proprietary systems or do not follow a standardized format and semantic annotation. The lack of open-access harmonized data limits the creation of transferable AI models and hinders benchmarking across systems and technologies [70].

Yet another significant issue is the explainability and robustness of AI models that are applied to critical infrastructure. Hydrogen systems have highly dynamic and safety-critical operating conditions, so AI-generated decisions must be explainable and trustworthy. Black-box models like deep neural networks are efficient but hard to interpret and tend to fail silently for unseen input conditions. This creates issues for their use in systems where human operators or regulators need traceable and auditable decision-making. Novel methods in Explainable AI (XAI), uncertainty quantification, and hybrid physics-informed machine learning provide possible solutions but remain unexplored in the context of hydrogen systems.

Interoperability and system integration also pose additional challenges since hydrogen is more deeply integrated into greater networks of renewable energy and industry [71]. Hydrogen technologies need to communicate with solar, wind, grid infrastructure, fuel cells, storage devices, and control systems that can employ varying communication protocols and data formats. The absence of common architectures and application programming interfaces (APIs) hinders end-to-end interoperability and reduces the potential of AI-based coordination [72]. To address this, future studies need to work towards creating modular and interoperable platforms where AI models can run across distributed energy systems without compromising scalability or reliability. Cybersecurity is also an increasing issue in AI-powered hydrogen infrastructure. With increasing digitization and dependency on cloud and edge computing in hydrogen systems, they expose themselves to cyber-attacks that can attack both data integrity and physical security [73]. There have been limited studies so far that have explored adversarial robustness, secure data exchange, or anomaly detection for hydrogen-specific cyber-physical systems. Therefore, an urgent need for the creation of secure architectures for AI that can function under limited conditions and protect against shifting threat vectors [74]. Figure 8 portrays a qualitative risk matrix outlining technical, operational, and regulatory risks related to AI deployment in hydrogen systems. The matrix allows for the identification of the various risks according to the amount of their impact and probability of occurrence, which gives the most prominent concerns such as data shortage, incompatibility between different systems and security weaknesses. The risks, which are considered to have a high impact on the hydrogen infrastructure, have to be resolved right away through explainable AI, and secure digital architectures. The medium-impact risks like the lack of standardization and the untrained workforce suggest that these are the areas where policy development and capacity building efforts should be coordinated. The risk matrix can be seen as a decision-support tool that helps with the prioritization of research and the guiding of the adoption of AI-enabled hydrogen technologies that are safe, scalable and trustworthy.

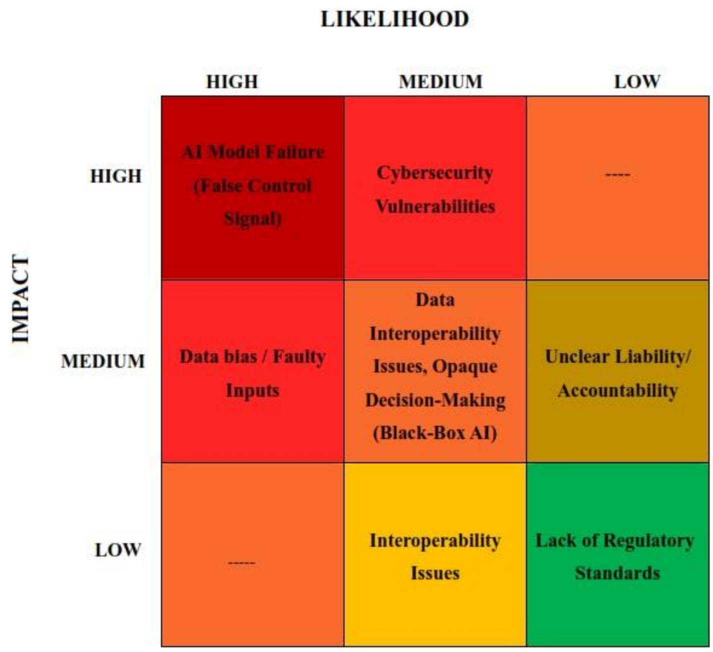

Figure 8. Risk Matrix for AI Deployment in Hydrogen Systems

From the systems point of view, there is also insufficient integration of comprehensive techno-economic models that embed AI-facilitated hydrogen systems within overall decarbonization plans. While AI can maximize single components or subsystems, its contribution to system-level trade-offs, like cost *vs.* carbon intensity, reliability vs. social acceptance, and the like, is not well modelled. Future research should thus focus on creating integrated models of assessment that analyze the effect of AI on the levelized cost of hydrogen (LCOH), carbon abatement potential, as well as the resilience of energy systems under various regional and policy scenarios. Lastly, building a talent pool skilled in working at the nexus of hydrogen engineering and AI is critical to maintaining long-term innovation. Training and education schemes need to shift to prepare energy professionals with data science, systems modelling, cybersecurity, and AI ethics competencies, while AI experts need to gain domain knowledge of hydrogen systems and sustainability challenges.

Based on these remarks, further research must emphasize the development of open-access, hybrid interpretable AI model design, modular and secure system and the integration of AI into policy-effective energy system models. Multidisciplinary collaboration between energy engineers, data scientists, policy specialists, and industry experts will be critical to make rapid progress in this new field. Table 7 outlines major identified research gaps in existing AI-hydrogen applications and suggests future directions to enhance system-level influence and scalability. By surmounting these obstacles, AI-based green hydrogen systems can transition from theoretical promise to practical effect, enabling the global ambition for a net-zero energy future.

Table 7. Research Gaps and Future Opportunities for AI in Hydrogen Systems

Hydrogen System Component	Current Limitation	Proposed AI Intervention	Future Research Direction	Potential Impact
Electrolyzers	Poor performance under fluctuating input	Reinforcement learning for dynamic control	Transfer learning for generalized control agents	High
Storage (e.g., hydrides)	Slow and costly material screening	ML-driven materials discovery	Integration with high-throughput simulations	High
Hydrogen logistics	Sub-optimal routing and scheduling	AI-based route optimization	Real-time, adaptive multi-agent coordination	Medium
Sectoral deployment	Low demand-side forecasting precision	Hybrid AI forecasting models	Cross-sectoral demand prediction platforms	High

7. CONCLUSION

Integrating artificial intelligence into green hydrogen systems thus marks a consequential innovation in achieving sustainable and decarbonized energy infrastructures. While countries and industries work on climate targets and reducing fossil fuel dependency, green hydrogen is a feasible energy vector that can sustain large-scale renewable energy deployment, storage of energy, and decarbonization across sectors. Unfortunately, inherent complexities in hydrogen systems, including fluctuating input conditions, nonlinear process dynamics, and different environments in which these systems can be applied, require more advanced tools for optimization, predictive control, and intelligent operation.

This review has explored the multiple uses of AI applied to the green hydrogen value chain from hydrogen production to storage and transportation. It has emphasized the various methods and techniques in AI, machine learning, deep learning, reinforcement learning, and DTs that can be applied to increase electrolyzer efficiency and hydrogen logistics optimizations. AI has a great scope in coordinating renewable-hydrogen hybrid systems and enabling intelligent energy management platforms for transport, power, and industrial sectors. Despite these encouraging advances, the general deployment of AI in hydrogen systems remains at an infancy stage and is confronted with several key impediments. These bottlenecks are presented by data, limitations of availability and quality, the need for explainable and robust models, and interoperability issues. Concerns for cybersecurity and the establishment of standards for infrastructure may add to these hurdles. In short, addressing these challenges will require an open-access data ecosystem, hybrid-AI models with physical constraints, and secure-modular digital infrastructure that can facilitate distributed intelligence .

Looking forward, future research must emphasize the coalescence of AI and hydrogen within large-scale energy system modelling networks, considering economic, environmental, and social dimensions. Through the combined synergy of artificial intelligence and green hydrogen, the energy industry can move toward a low-carbon, efficient, and resilient future.

Declarations of interest

The authors declare no conflict of interest in this reported work.

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